

Diagonalization in Reduced Hilbert Spaces using a Systematically Improved Basis: Application to Spin Dynamics in Lightly Doped Ladders

E. Dagotto¹, G. B. Martins¹, J. Riera², A. L. Malvezzi¹, and C. Gazza¹

¹ *National High Magnetic Field Lab and Department of Physics, Florida State University, Tallahassee, FL 32306*

² *Instituto de Física Rosario, Avenida Pellegrini 250, 2000 Rosario, Argentina*

A method is proposed to improve the accuracy of approximate techniques for strongly correlated electrons that use reduced Hilbert spaces. As a first step, the method involves a change of basis that incorporates exactly part of the short distance interactions. The Hamiltonian is rewritten in new variables that better represent the physics of the problem under study. A Hilbert space expansion performed in the new basis follows. The method is successfully tested using both the Heisenberg model and the $t - J$ model with holes on 2-leg ladders and chains, including estimations for ground state energies, static correlations, and spectra of excited states. An important feature of this technique is its ability to calculate dynamical responses on clusters larger than those that can be studied using Exact Diagonalization. The method is applied to the analysis of the dynamical spin structure factor $S(\mathbf{q}, \omega)$ on clusters with 2×16 sites and 0 and 2 holes. Our results confirm previous studies (M. Troyer, H. Tsunetsugu, and T. M. Rice, Phys. Rev. **B53**, 251 (1996)) which suggested that the state of the lowest energy in the spin-1 2-holes subspace corresponds to the bound state of a hole pair and a spin-triplet. Implications of this result for neutron scattering experiments both on ladders and planes are discussed.

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I. INTRODUCTION

The study of strongly correlated electrons is currently among the most active areas of research in condensed matter physics. In recent years the discovery of a variety of new phenomena such as high temperature superconductivity, buckyballs, and colossal magnetoresistance effects [1] have triggered a huge theoretical effort devoted to the analysis of the electronic models proposed for these compounds. Since experimental data suggests that the electronic interactions cannot be considered as small perturbations in the typical regime of couplings of these models, the use of nonperturbative techniques, especially computational ones, has become a popular approach for the study of complicated many-body problems in the area of materials research.

In spite of their popularity, numerical methods are not without problems. The well-known Lanczos approach [2] provides exact static and dynamical information for finite clusters. However, current memory limitations in available computers constrain the cluster sizes that can be studied. An alternative is the same Lanczos method but now applied on a reduced basis set. However, experience has shown that the convergence to accurate results is slow, at least for the basis expansion procedures proposed thus far [3,4]. Recently, the Density Matrix Renormalization Group (DMRG) has been introduced [5] providing an optimal way to perform a basis expansion in quasi-one dimensional systems. The method certainly gives accurate results in the study of equal-time correlations for a variety of models, but currently it does not provide dynamical information and since it is typically

applied on open boundary clusters the study of the momentum dependence of observables is complicated. Alternative techniques such as the Quantum Monte Carlo algorithm [6], where a guided sampling of configurations is carried out, can handle medium size clusters but it fails at low temperatures due to the “sign problem”.

Some of the complications of these algorithms can be traced back to the important differences between the degrees of freedom used explicitly in the construction of the Hamiltonians, and those that are dynamically generated in the solution of the problem. A typical example is provided by the problem of holes close to half-filling in the $t - J$ model: the eigenstates are made out of a hole (empty site) plus a surrounding cloud of spin distortions that carry the actual quasiparticle spin. Depending on parameters the quasiparticle size can involve dozens of sites, and thus it differs drastically from a bare one-site hole. It has been shown that the use of quasiparticle operators [7] provides more accurate information than other approximate methods based on the bare degrees of freedom. Note that the distinction arises from the approximate character of most calculations. If one were to solve the problems exactly, the results would be independent of the actual initial formulation of the problem.

The goal of the present paper is twofold. Motivated by the discussion above, first a computational method is discussed where the Lanczos method is applied on a reduced Hilbert space to allow for the study of clusters larger than those that can be handled exactly. To achieve this goal in an efficient way it is proposed to change the basis in which the problem is formulated to accelerate the convergence to ground state properties as the size of the

reduced basis grows (Sec.II). This basis can be improved systematically. The technique is tested in hole undoped and doped models (Sec.III). The main advantage of this method is that it provides dynamical information on intermediate size clusters. The second goal of the paper is to apply this technique to the study of the dynamical spin structure factor of doped 2-leg ladder systems (Sec.IV). Clusters with 2×16 sites and 0 and 2 holes were analyzed. In agreement with previous studies [8], it is here observed that the excitation of lowest energy in the subspace of 2 holes and spin-1 corresponds to the bound state of the 2-holes pair (which already exists in the spin-0 sector) and a spin-triplet. Implications of this result for neutron scattering experiments in both ladders and planes are briefly discussed (Sec.IV.B).

II. METHOD

As discussed in the Introduction, one of the purposes of this paper is to propose an improvement on the method of diagonalization in reduced Hilbert spaces [9]. This method usually has the problem that the convergence to an accurate result is slow as the reduced Hilbert space size grows [3,4]. This complication may be caused by the improper selection of the basis in which the problem is formulated which, thus far, has been suggested mainly by the actual form of the Hamiltonian. To improve on this approach let us consider as example the $t - J$ model on a 2-leg ladder. This system is currently widely studied both theoretically and experimentally due to the presence of a robust spin gap in the spectrum and superconductivity upon doping [10]. In the context of ladders it is easy to construct a good basis for the ground state. In fact several studies have observed that the ground state of ladders in the realistic regime where the chain (J) and rung (J_\perp) couplings are similar and at low hole-density is qualitatively related to the ground state in the large J_\perp/J limit, which is formed by the direct product of rung singlets [10]. This information suggests that the use of a “rung” basis (made out of a singlet and a triplet per rung in the hole undoped case) would be more suitable than the standard so-called S^z -basis of spins up and down at each site [11]. The case of large J_\perp/J makes this statement more clear: in the S^z -basis, and working on an undoped $2 \times L$ ladder, 2^L states are still needed for the ground state. However, in the rung-basis the same ground state is represented by just *one* state which is the configuration with singlets at every rung. As the ratio J_\perp/J decreases more states will be needed for the ground state to reach a given accuracy in the energy or correlations, but it is expected that their number will remain smaller than those needed in the S^z -basis.

Although the basic idea of improving the basis in which a problem is formulated has been used before in several contexts, such as in Physical Chemistry, its application to problems of strongly correlated electrons has been more

limited. The DMRG technique mentioned before is an approach in the same spirit, improving the basis used in the problem at hand, and it is applied mainly to systems with open boundary conditions. The method described in the present paper is a complement to such previous efforts, and provides an alternative technique that allows for the calculation of dynamical information and momentum dependent observables.

The method certainly goes beyond the mere change from the S^z -basis to the rung-basis described in the previous paragraph. For instance, still in the context of ladders it is natural to continue increasing the size of the clusters which are considered exactly in the construction of the new basis. Next in line is the plaquette basis built upon the exact solution of a 2×2 cluster [12] (see Fig.1a). Certainly the plaquette basis will be even better than the site- and rung-basis since extra short distance correlations are treated exactly in the problem. In the plaquette basis the diagonal energies ϵ_d range from $-2J$ to J (for an undoped plaquette), and it is expected that the states will have a smaller contribution to the ground state as their energies ϵ_d move away from $-2J$. Numerically the procedure can be continued using exactly solvable clusters of increasing size.

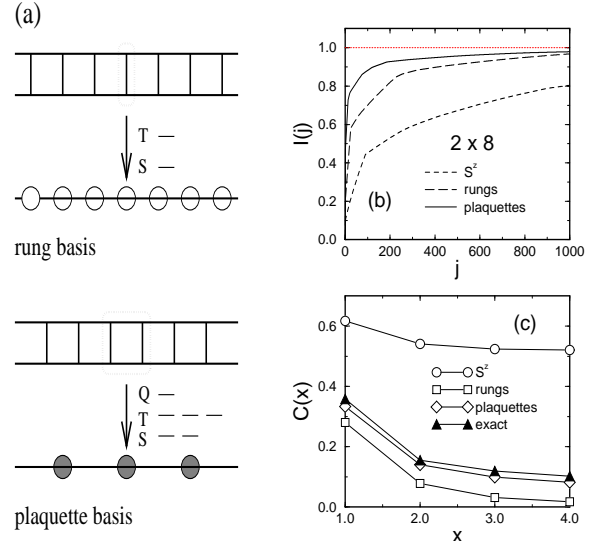


FIG. 1. (a) Schematic representation of the change of basis to rungs and plaquettes for an undoped system. Shown also schematically are the states for each basis with their spin (S, T, and Q, denote a singlet, triplet, and quintuplet, respectively, and the short segments next to them denote their number in the basis under discussion, not their energy); (b) Integrated weight $I(j)$ (see text) vs j , index that labels the states ordered sequentially from large to small according to their weight in the exact ground state of an undoped 2×8 cluster. Shown are results for three basis; (c) Staggered spin-spin correlation $C(x)$ for the same 2×8 cluster using the 2^8 states which have the highest weight in the exact ground state for the three basis indicated, compared with the exact results obtained with the total 12,870 states.

The same reasoning can be applied to other spin models such as those corresponding to dimerized chain systems where the natural basis is made out of singlets and triplets in the “strong” bonds. In 1D electronic and spin Hamiltonians, a good basis arises from solving exactly $1 \times L$ small segments, as shown explicitly below. The same is true whether one- or three-band Hubbard models are considered. The physics of 2D systems can be approached by the study of N -leg ladders with increasing value of N , as recently proposed in DMRG calculations [13]. In this case the block that should be solved exactly is the generalized N -site rung. Thus, by no means the approach presented here is restricted only to ladders, but it is general and independent of the cluster geometry and model (results in 2D will be presented in future publications). In general, the goal is to consider exactly at least part of the *short* distance correlations by a suitable change of basis, and then carry out some other numerical or analytical approximate technique to complete the calculation for a given accuracy in observables. By changing the basis a better starting point for most many-body approximate techniques will be achieved [14]. Although it is unlikely that in quasi-1D systems the method will be more accurate than the DMRG technique for equal-time correlations, nevertheless it can produce dynamical and momentum dependent correlations and in this respect it is a complement to previous DMRG and Lanczos approaches.

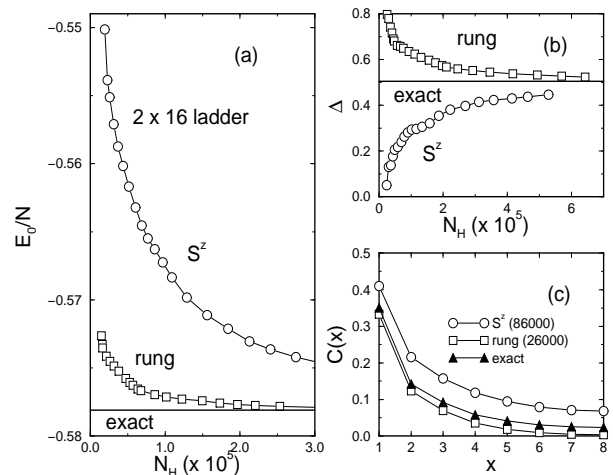
III. TESTS OF THE TECHNIQUE

A. Undoped Systems

Fig.1b illustrates the advantages of using basis that diagonalize exactly a small cluster over the S^z -basis for the case of a small undoped ladder. Diagonalizing the Heisenberg Hamiltonian for the 2×8 cluster in the three considered basis, the 12,870 states were sequentially ordered from large to small according to their weight in the normalized exact ground state. The integrated weight $I(j) = \sum_{i=1}^j |c_i|^2$, where c_i is the coefficient of the i -th state in the ground state, provides information on the weight distribution. A rapid convergence to 1 implies that a small subset of the basis can carry an important fraction of the total probability. In agreement with the previous discussion the convergence is rapidly improved as the size of the cluster exactly considered in the basis increases. For instance, to reach 90% of the total weight the plaquette basis needs about 150 states, while in the S^z -basis over 2,000 states are required (results as encouraging as these ones are shown below also for 1D systems and doped ladders). Larger clusters beyond plaquettes would improve even further this result.

1. Equal-time Spin Correlations

This basis-dependent redistribution of weight has consequences for the calculation of expectation values when only a fraction of the total Hilbert space is used. As example consider the staggered spin-spin correlations defined as $C(x) = (1/N) \sum_y (-1)^x \langle \mathbf{S}_y \cdot \mathbf{S}_{y+x} \rangle$ (standard notation) which are of special importance since their long distance behavior reflects on the gapless vs gapped character of the energy spectrum. It would be desirable that a reduced basis provides a qualitatively correct $C(x)$ at large distances. Considering only the 256 states with the largest coefficients for the 2×8 ladder, Fig.1c shows that the S^z -basis gives a staggered spin correlation too large compared with the exact result. This problem occurs because the states with the largest ground state weight in this basis are small modifications around the pure Néel state which has staggered order. On the other hand, using the basis that diagonalize blocks with 2 and 4 sites considerably better results are achieved with the same computational effort since the dominant state in the rung-basis (singlets in all rungs) already has a robust spin-gap as the exact ground state of the 2-leg ladder.



[†] FIG. 2. (a) Ground state energy per site E_0/N (in units of J) vs size of the reduced Hilbert space N_H for the Heisenberg model on a 2×16 ladder using the S^z - and rung-basis. The exact (Lanczos) result is -0.5781032 ; (b) Spin-gap vs N_H on an undoped 2×16 ladder using the S^z - and rung-basis. The exact result 0.505460384 is also shown. Each point represents the difference between the energies of the lowest energy state in the subspaces of spin-1 and -0 for a given size of the Hilbert space common to both subspaces; (c) Staggered spin-spin correlation $C(x)$ for the 2×16 cluster. Results in the S^z -basis (rung-basis) were obtained using $\sim 86,000$ ($\sim 26,000$) states. The exact results were obtained with the Lanczos method.

In Fig.2a the evolution of the ground state energy as the dimension of the reduced Hilbert space grows is

shown for the S^z - and the rung-basis using now an undoped 2×16 cluster. A considerably faster convergence is achieved with the latter producing 4 significant figures in the energy with only 300,000 states ($\sim 1.6\%$ of the total space). The details of the expansion procedure are independent of the basis used, and since they are described in previous literature they will not be repeated here [4]. Similar rapid convergence is achieved if the energy of the first excited state of spin 1 and momentum (π, π) is investigated (Fig.2b). Regarding $C(x)$ the behavior on the undoped 2×16 cluster (Fig.2c) resembles results on smaller systems: better correlations are obtained with the rung-basis even if less states are used than in the S^z -basis.

The algorithm described in this paper is used for clusters with periodic boundary conditions, and thus it is possible to carry out the basis expansion procedure in a basis of momentum eigenstates. This allows us to gather information about, e.g., excited states of spin 1 with different momenta which is important to compare results against those obtained with inelastic neutron scattering techniques. Results for the Heisenberg model are given in Fig.3a. Once again using a small fraction of the total space and the rung-basis accurate energies are obtained at all momenta for this cluster. The results are in excellent agreement with previous predictions by Barnes and Riera [15].

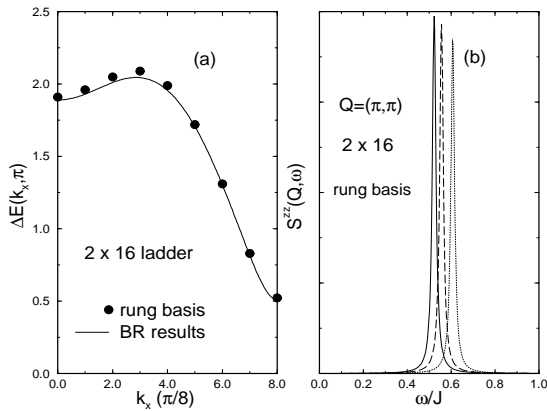


FIG. 3. (a) Energy gap between the state of lowest energy in the subspace of spin-1 and momentum- \mathbf{q} and the ground state for the Heisenberg model, using $\sim 300,000$ rung-basis states in each subspace. The rung momentum is fixed to π . Results are compared against the calculations of Barnes and Riera (BR) (b) Dynamical spin structure factor $S^{zz}(\mathbf{Q}, \omega)$ with $\mathbf{Q} = (\pi, \pi)$. Dotted, dashed, and solid lines indicate results using 120,000, 253,000, and 410,000 states in the reduced Hilbert space of spin-1 and momentum \mathbf{Q} obtained after the application of the $S_{\mathbf{Q}}^z$ operator over a reduced ground state with about 50,000 rung-basis states. The latter was obtained from an approximate overall ground state (spin-0) of about 600,000 rung-basis states.

2. Dynamical Spin Structure Factor

An interesting advantage of the method proposed here is that having a good approximation to the ground state expressed in a simple enough basis allow us to obtain *dynamical* information without major complications. In other techniques the ground state is either lost in the iterative processes, or it is expressed in a cumbersome basis for the application of the operator being investigated (spin, charge, current) over such ground state. As example, here the dynamical spin structure factor $S^{zz}(\mathbf{q}, \omega)$ was calculated. The actual procedure is simple: the operator $\hat{O} = S_{\mathbf{q}}^z$ (standard notation) is applied to the ground state in the reduced basis denoted by $|\phi_0\rangle_T$. If all states of the subspace of spin-1 and momentum \mathbf{q} generated by the operation $\hat{O}|\phi_0\rangle_T$ were kept in the process, typically one would exceed the memory capabilities of present day workstations if the truncated ground state has about 3×10^6 states. Then, it is convenient to work with just a fraction of $|\phi_0\rangle_T$, say keeping about 10% of the states. In this way the subspace of spin-1 under investigation typically has a similar size as the original reduced basis ground state, namely approximately 3×10^6 rung-basis states. The state $\hat{O}|\phi_0\rangle_T$ constructed by this procedure is now used as the starting configuration for a standard continued fraction expansion generation of the dynamical response associated to \hat{O} [2]. As a test results are shown in Fig.3b for an undoped 2×16 cluster and $\mathbf{q} = (\pi, \pi)$. As observed in the figure, for the case of the undoped 2-leg ladder $S^{zz}(\mathbf{q}, \omega)$ is dominated by just one peak with small weight at higher energies. The convergence as the reduced basis set grows is fast, and the results are quantitatively accurate even with only $\sim 1\%$ of the total space in the ground state. Results at other momenta and for doped ladders behave similarly and they will be analyzed later in Section IV.

3. Results for Intermediate Size Clusters

Fig.4 contains $C(x)$ for the Heisenberg model on a 2×20 cluster, which cannot be studied exactly. Using up to $\sim 1,600,000$ states (just 0.04% of the total space) the results for $C(x)$ are in good agreement with world-line Monte Carlo simulations at low temperatures. The ground state energy is obtained with three significant figures using this basis set. The existence of a short antiferromagnetic correlation length ξ_{AF} [10,16] is clear from Fig.4, and in this respect the basis expansion method in the rung-basis has captured properly the qualitative aspects of the ladder ground state, which are dominated by short-range antiferromagnetic fluctuations and rung singlet formation. Similar calculations in the S^z -basis keeping the same number of states incorrectly suggest that ξ_{AF} is very large. In addition, note that there are undoped ladder compounds, such as $\text{Cu}_2(\text{C}_5\text{H}_{12}\text{N}_2)_2\text{Cl}_4$, that are highly anisotropic with $J_{\perp}/J = 5.5$ [17]. In this

regime the rung-basis is particularly useful: combining information from exactly solvable clusters and Lanczos in a reduced rung-basis set for larger systems, the spin-gap for $J_{\perp}/J = 5.5$ was accurately found to be 4.598105.

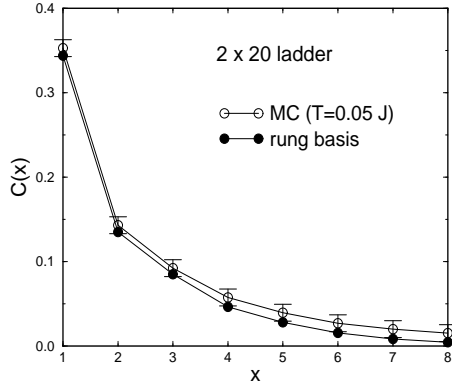


FIG. 4. Spin correlation $C(x)$ vs x for a 2×20 Heisenberg cluster obtained keeping 1,600,000 states in the reduced basis (0.04% of the total Hilbert space), compared with world-line Monte Carlo results for the same cluster at temperature $T = 0.05J$.

B. Doped systems

The method proposed here certainly applies to hole doped (fermionic) systems, and to models in geometries different from ladders. To illustrate these cases in Fig.5a-b results are presented for (i) a 1D $t - J$ chain with 2 holes using as basis the states that diagonalize exactly blocks of 2 and 4 sites, and (ii) an anisotropic ladder with 1 hole using the rung basis (and with an anisotropy corresponding to the region where pairing correlations are maximized upon further doping [18]). The advantage of using these new basis is clear from the figure. For the anisotropic ladder 80% of the weight is obtained with 15 states in the rung-basis, compared with 350 in the S^z -basis. In addition, Fig.5c shows results for the $t - J$ model with 2 holes on a 2×16 cluster that cannot be studied exactly. Using $\sim 500,000$ rung-basis states a ground-state snapshot is provided in Fig.5c where one hole is projected to be at an arbitrary site and the probability of finding the second hole at some other site is presented. The results illustrate the formation of two-hole bound states and they are in excellent agreement with those previously reported using other techniques [13,19]. Then, it is concluded that the method discussed in this paper can handle properly systems with holes, in addition to undoped spin models.

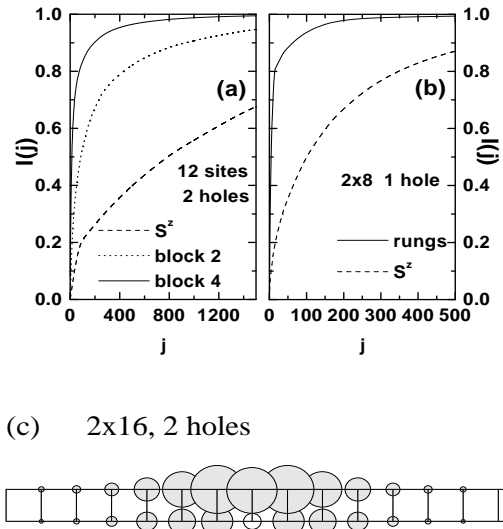


FIG. 5. (a) $I(j)$ vs j (see Fig.1b) using the exact ground state of the $t - J$ model on a 12-site chain with 2 holes at $J/t = 0.4$. The basis are the standard S^z , and the 2-block and 4-block basis where the exact solutions for clusters of 2 and 4 sites are used; (b) $I(j)$ vs j using the exact ground state of the $t - J$ model on a 2×8 anisotropic ladder with $J/t = 0.4$, $t_{\perp}/t = 1.5$, $J_{\perp}/t = 0.9$ and 1 hole. Results for the S^z - and rung-basis are shown; (c) Distribution of holes for the $t - J$ model on a 2×16 cluster with 2 holes at $J/t = 0.4$ using $\sim 300,000$ rung-basis states. The area of the gray circles at a given site are proportional to the probability of finding a hole at that site, once the other hole is fixed at an arbitrary position (open circle)

IV. DYNAMICAL SPIN STRUCTURE FACTOR IN DOPED LADDERS

A. Results and Interpretation

As an application of the technique presented in the previous Sections, here an analysis of $S(\mathbf{q}, \omega)$ will be reported for lightly doped 2-leg ladders. The study is performed on clusters of size 2×16 which cannot be studied exactly. Previous work in this context discussed an interesting property of the subspace of spin-1 in doped ladders [8]. The overall ground state in this subspace corresponds either to two unbound hole quasiparticles (each carrying a spin-1/2) or to a *bound* state of a hole pair (similar to the pair that appears in the ground state of the 2-holes spin-0 subspace [10]) and a spin-triplet. This result should be contrasted against the ground state of the spin-1 sector in undoped ladders which in the limit of a large rung exchange J_{\perp} simply consists of one spin-triplet at an arbitrary rung and spin-singlets in all the other rungs. Such a result suggests that in doped ladders with 2 holes the state with a tight hole-pair separated in space from the rung-triplet would contribute

substantially to $S(\mathbf{q}, \omega)$. This is indeed true and the spin dynamical structure factor is dominated by such a configuration. However, the state where the pair and the spin-triplet are bound has a lower energy and it is expected to generate a low-intensity branch of excitations in the spectrum of lightly doped ladders, below the high-intensity branch that evolves smoothly from the undoped limit [8].

In Fig.6, $S(\mathbf{q}, \omega)$ is presented on a 2×16 cluster with no holes, and using the technique described in this paper. In this study efforts are concentrated on the $q_y = \pi$ branch which is the most interesting for the physics of the problem. The spin-0 ground state has here $\sim 10^6$ states, of which the dominant $\sim 150,000$ were used in the dynamics. The subspace obtained by the application of the $S_{\mathbf{Q}}^z$ operator over this state also has approximately 10^6 rung-basis states. A clear peak can be observed in the figure at all momenta, with a pole energy position already provided in Fig.3a. The largest weight is obtained at momentum (π, π) .

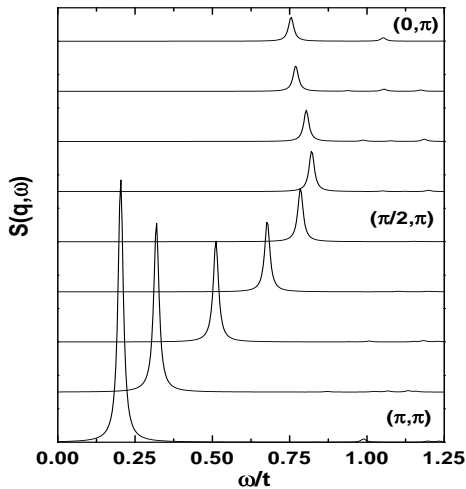


FIG. 6. $S(\mathbf{q}, \omega)$ for the $q_y = \pi$ branch on a 2×16 cluster with no holes. The technique used is the method proposed here in Sec.II. The number of states in the reduced basis is explained in the text. The δ -functions have been given a width $0.01t$.

Fig.7 contains a similar result but now in the sector of 2 holes using $\sim 3 \times 10^6$ rung-basis states for the spin-0 ground state, of which $\sim 150,000$ are kept for the dynamics. The subspace of 2 holes, spin-1 and momentum \mathbf{q} typically has also $\sim 3 \times 10^6$ states. The spectrum has two main branches: (I) is the branch with the highest intensity and it is in good correspondence energy- and shape-wise with the result in the undoped limit. As explained before, these states are expected to correspond to a tight pair of holes plus a spin excitation, separated spatially from the first (i.e. without forming a bound

state); (II) corresponds to the actual ground state of the subspace of spin-1 at all the momenta investigated here. This state is expected to be a bound state between a hole-pair and a spin excitation. Note that symmetry considerations [8] explain why branch (II) has zero weight at momentum (π, π) . The reason is that with two holes the actual lowest-energy state of spin-1 is exactly orthogonal to the state obtained from applying $S_{\mathbf{Q}}^z$ to the spin-0 2-hole ground state. These states transform differently under reflections along the ladder direction. Such an effect is expected to disappear for a larger number of holes. In spite of this orthogonality problem, the position of the bound state pair-triplet at momentum (π, π) can be obtained using other techniques. For instance, using the DMRG method on a 2×16 cluster with periodic boundary conditions, 2 holes, total z -projected spin one, and $J/t = 0.4$ it was found that the spin-gap is $\sim 0.26t$ ($m = 200$, truncation error 5×10^{-5}). Information about this gap can actually also be found in the continued fraction expansion procedure to obtain Fig.7 since a pole with negligible weight nevertheless appears in the process. Its position is very similar to the result found with DMRG.

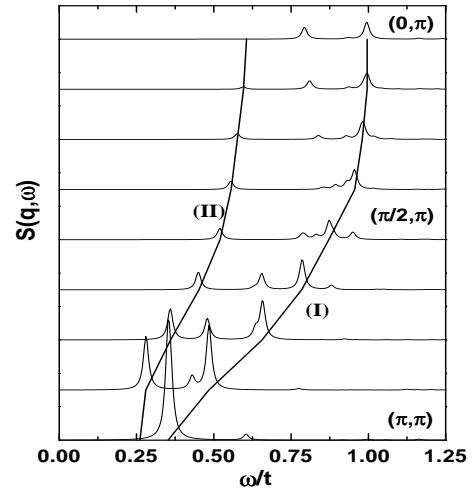


FIG. 7. Same as Fig.6 but for the case of a 2×16 ladder with two holes. The physical meaning of branches (I) and (II), as well as the number of states used in the study, are explained in the text.

To verify in more detail the physical interpretation of branch (II), the ground state of an 2×8 cluster was obtained exactly using the Lanczos algorithm working in the rung-basis. The dominant configuration in the limit where J_{\perp} is the largest scale is shown in Fig.8a (using as example $J_{\perp}/J = 10$, $J/t = 0.4$, and hopping amplitudes $t = 1$ along both rungs and legs). This state has two holes in the same rung, and a rung-triplet right next to

the pair (of course the state with the triplet on the other side of the pair carries the same weight). The next dominant state is shown in Fig.8b and it corresponds to having nearest-neighbor rungs with one hole and a spin up each. The overall $q_y = \pi$ momentum is obtained by using one hole with rung-momentum 0 and the other with π . The combination of the states Fig.8a and 8b (and the other two obtained by reflections along the legs) carry 74% of the weight of the ground state in this large J_\perp example. The fact that both the pair of holes and the spin-1 are located spatially close to each other indicates that a bound state pair-triplet has been formed, as anticipated.

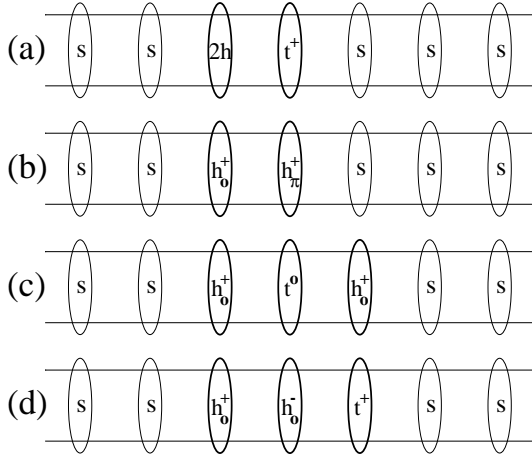


FIG. 8. (a) Dominant configuration in the rung-basis corresponding to a 2×8 ladder with $J_\perp/J = 10$, $J/t = 0.4$, and hopping amplitudes $t = 1$ along both rungs and legs; (b) Next dominant configuration for the same parameters as in (a); (c) Dominant configuration for the isotropic case $J_\perp/J = 1.0$, with all other parameters as in (a); (d) Next dominant configuration for the parameters of (c). Both in (c) and (d) the results are the same for 2×8 and 2×16 clusters. The convention followed here is the following: s denotes a spin singlet along the rung, t^+ is a rung-triplet with z -projection $+1$, t^0 is a rung-triplet with z -projection 0, $2h$ is the state of two holes in the same rung, and h_0^+ and h_π^+ are the rung-states of one hole with spin-up and momentum 0 and π , respectively.

Fig.8c shows the dominant configuration for the more realistic case of $J_\perp = J = 0.4$ and $t = 1$. The holes forming the pair are now located at a distance of two lattice spacings along the legs, with a spin-triplet in between. In the next dominant configuration (Fig.8d) the holes are separated by one lattice spacing, with the triplet on the side. These states still represent the bound state pair-triplet observed at large J_\perp and predicted in Ref. [8]. The main differences between Figs.8a-b and c-d simply originate in the fact that the bound state is more extended in the rung-leg isotropic limit than in the $J_\perp \gg J$ case. It is interesting to observe that these configurations are also dominant for larger clusters. Actually the expansion procedure described in this paper was applied to the 2×16 cluster, in the spin-1 subspace, with mo-

mentum (π, π) , keeping about 10^6 states. The dominant rung-basis states were found to be the *same* as shown in Figs.8c and d. Note also the clear advantage of using the rung-basis in this visualization of dominant configurations: the state of Fig.8a expressed on a 2×16 cluster and using the S^z -basis would require $2^{14} = 16,384$ states.

B. Implications for Neutron Scattering Experiments

1. Ladders

The results of the previous subsection have implications for neutron scattering experiments on ladder compounds. Although the study of ladder materials with neutron scattering techniques has been restricted thus far to the undoped limit [20], experiments for doped ladders $\text{Sr}_{14-x}\text{Ca}_x\text{Cu}_{24}\text{O}_{41}$ are being planned [21]. In this context, experimentalists should observe two branches in their spectra, namely (I) and (II) of Fig.7. Branch (II) has an intensity that grows with the number of holes, and thus naively it is expected to be weak. However, note that in Fig.7 and considering momentum $\mathbf{q} = (7\pi/8, \pi)$, the weights of both branches (I) and (II) are *similar* in intensity, even in a situation where the nominal density is as small as $x = 2/32 = 0.0625$. Thus, the experimental search for branch (II) may not be difficult, and its observation would provide support to calculations that predict the formation of tight pairs in 2-leg ladders [10].

2. Planes

Note that excitations such as those corresponding to branch (II) could appear also in the two-dimensional high-Tc cuprates. It is well-known that these materials present a pseudogap behavior in the underdoped regime. Some theories explain this feature as caused by magnetic effects [22], while others attribute its origin to preformed hole pairs [23]. A mixture of these two proposals was recently introduced using results on ladders as a guidance [24]. In this context it was suggested that the short-range antiferromagnetic (AF) order of lightly doped cuprates may lead to long-lived hole-pairs in the normal state. These pair may cause several anomalies in transport, neutron, and photoemission experiments. In this framework the pseudogap is correlated with the existence of a finite AF correlation length, which is necessary to form the pairs.

In Ref. [24] the spectral function of doped ladders for up to 2×20 sites clusters was presented. A gap at $(\pi, 0)$ was clearly observed due to the existence of tight pairs on ladders. Analyzing the same $t - J$ ladder model and hole density, both in Ref. [8] and here it has been observed that having a state with tight hole pairs have important consequences not only for photoemission experiments but also for neutron-scattering experiments since

in this context a new branch in the spectra should be observed (tight spin-triplet hole-pair). Note that the effect discussed here is not caused by any bilayer structure as some theories propose [25], but it is expected to appear in isolated copper-oxide planes as well. Also there is no need to fine tune parameters in the $t - J$ model to observe the states describe in this section, which exist in a wide region of parameter space.

These novel excitations may have already been observed in the broad normal state peaks of underdoped YBCO reported recently [26], related to the famous resonances in the superconducting state of optimally doped YBCO [27], but certainly considerable more work is needed to relate the present ideas with experiments. It also remains to be investigated what is the relation between the bound pair-triplet excitation branch (II), and other theories for the sharp peaks in neutron scattering that appear in cuprates, such as the collective modes in the particle-particle channel [28] and the spin-wave excitation explanation [29].

V. SUMMARY

Summarizing, here it was proposed that the accuracy of some approximate techniques for the study of many-body problems, such as the Lanczos approach in a reduced basis, can be improved if a change of basis is performed that incorporates exactly short distance interactions in the problem. Numerical methods using reduced Hilbert spaces converge faster in the new basis than in those naively suggested by the degrees of freedom explicit in the Hamiltonian. The method described here is certainly in the same spirit as previous techniques that also improve systematically the basis used in a given problem, such as the DMRG method. The advantage of the approach discussed here is that it allows for the calculation of dynamical information on clusters larger than those that can be solved exactly. Although the technique was tested only on undoped and doped ladder and chains systems, the approach can be used for a wide variety of problems independent of their dimension and geometry, and for both doped and undoped systems. Analytic techniques, such as perturbation theory, can also improve their convergence radius using a better basis [30].

In addition, in the present paper the dynamical spin structure factor $S(\mathbf{q}, \omega)$ was calculated for lightly doped ladders. In agreement with previous literature [8], a low-intensity branch was observed away from half-filling. This branch appears at an energy smaller than the high-intensity branch that smoothly evolves from the undoped system. This new branch is characteristic of systems with tight hole pair bound states, and it should be detectable in neutron scattering experiments for ladders. If hole pairs (or long-lived pairs) exist in the normal state of the underdoped two-dimensional cuprates, such an excitation could be detectable also in this context.

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